On the zero mass limit of tagged particle diffusion in the 1-d Rayleigh-gas

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February 2, 2008

Dedicated to Domokos Szász on his 65th birthday

Abstract

We consider the $M \to 0$ limit for tagged particle diffusion in a 1-dimensional Rayleigh-gas, studied originaly by Sinai and Soloveichik [14], respectively by Szász and Tóth [19]. In this limit we derive a new type of model for tagged paricle diffusion, with Calogero-Moser-Sutherland (i.e. inverse quadratic) interaction potential between the two central particles. Computer simulations on this new model reproduce exactly the numerical value of the limiting variance obtained by Boldrighini, Frigio and Tognetti in [4].

1 Introduction

The problem of deriving relevant information on the diffusive scaling limit of tagged particle motion (i.e. self-diffusion), from microscopic principles has been undoubtedly at the heart of mathematically rigorous statistical physics of time dependent phenomena, at least since Einstein's groundbreaking work. Mathematically rigorous investigation of tagged particle diffusion in systems of particles governed by deterministic (Hamiltonian) dynamics is notoriously difficult even in one dimensional models. After remarkable advances achieved up to the late 1980-s (see Section 3 below and references cited there), in the last twenty years there seemed to be less intense activity in the field. This is certainly due to the difficulty of these problems and lack of technical tools to attack them.

In the present note we make a small but hopefully not completely irrelevant contribution to the subject. We investigate the $M \to 0$ small mass limit of the tagged particle diffusion in the so-called 1-dimensional Rayleigh-gas. This system consists of an infinitely extended one-dimensional system of point-like particles of mass 1 and one single tagged particle of mass M immersed in it. The particles perform uniform motion and interact through elastic collisions. The system is distributed according to the equilibrium Gibbs measure. This means independent exponentially distributed inter-particle distances and independent normally distributed velocities with mean zero and inverse mass variances (that is: equidistributed kinetic energy). It is a fact that the dynamics of the infinitely extended system is almost surely well defined under this stationary measure. That is: no multiple collisions and no accumulation of infinitely many particles in finite time occurs. Randomness comes into the problem only through the thermal equilibrium of the initial condition, otherwise the dynamical evolution is deterministic. The central question is understanding the diffusive scaling limit of the trajectory of the tagged particle: $A^{-1/2}Q_{At}$, as $A \to \infty$. There exist a number of deep and interesting results related to this problem which will be shortly surveyed in Section 3. In the present note we investigate the limit when $M \ll 1$. We prove that in this limit the system becomes equivalent to another, new model of tagged particle motion, differing from the one described above in having instead of one central particle of different mass, all particles of the same mass but the two central particles interacting via a Calogero-Moser-Sutherland-type repulsive potential, with random strength parameter. This result explains some phenomena observed in earlier computer simulations on the Rayleigh-gas. In particular the instability observed for small values of M. We also present numerical simulations on this new model. Our simulation results reproduce very accurately the numerical value of the limiting variance of tagged particle in the Rayleigh-gas, in the $M \to 0$ limit, which were obtained in [4]. We claim that our result not only reproduces (from a completely different approach) the numerical value but also gives theoretical explanation of the phenomenon.

The paper is organised as follows: In Section 2 we define the models of interacting particle systems considered, their stationary Gibbs measures and the stochastic processes whose diffusive asymptotics is later analysed. In Section 3 we briefly survey the existing earlier results (rigorously proved and numerical, alike) on tagged particle diffusion in 1-d Rayleigh-gas. In Section 4 we properly state and prove the theorem which states that in the $M \to 0$ limit the 1-d dynamics of the Rayleigh-gas with tagged particle of mass M converges (trajectory-wise, in a natural topology) to the dynamics of the 1-d gas of particles with Calogero-Moser-Sutherland interaction between the two central particles. Finally, in Section 5 we present our new numerical results referring to this new type of interacting particle system. We should emphasize here that our numerical results are not just accurate reproduction of older computer experiments but are performed on a genuinely new type of model. One of the main points of this paper is exactly the fact that these genuinely new numerical results are in accurate agreement with the results of Boldrighini, Frigio, Tognetti [4], giving independent enhancement *and theoretical explanation* to them.

2 Models: state space, dynamics, stationary measures

In this section we describe the models considered throughout the paper. In section 2.1 we present a formal definition of the state spaces and the natural measures on them. Section 2.2, which gives a more verbal description of the time evolution in our dynamical systems, clarifies that these models indeed correspond to the one dimensional gases mentioned in the Introduction.

2.1 State spaces and stationary Gibbs measures

Let

$$\Omega^{\pm} := \{\omega^{\pm} = (x_{\pm i}, v_{\pm i})_{i=1}^{\infty} : (x_{\pm i}, v_{\pm i}) \in \mathbb{R}^{\pm} \times \mathbb{R}, \quad x_{\pm 1} = 0, \quad \pm(x_{\pm(i+1)} - x_{\pm i}) \geq 0\}.$$

With slight abuse of notation and terminology sometimes we don't distinguish between $\omega^{\pm}$ and the (unordered) set of points $\{(x_{\pm i}, v_{\pm i}) : i = 1, 2, \dots\} \subset \mathbb{R}^{\pm} \times \mathbb{R}$. We endow the spaces $\Omega^{\pm}$ with the topology defined by pointwise convergence: $\omega_n^{\pm} \to \omega^{\pm}$ iff $(x_{\pm i}, v_{\pm i})_n \to (x_{\pm i}, v_{\pm i})$, for all $i = 1, 2, \dots$. This is a metrizable topology and makes $\Omega^{\pm}$ complete and separable (i.e. Polish) spaces.

We denote by $\mu^{\pm}$ the following probability measures over $\Omega^{\pm}$, respectively. Under $\mu^{\pm}$ the random variables $\xi_{\pm i} := \pm\big(x_{\pm(i+1)} - x_{\pm i}\big)$, $\eta_{\pm j} := v_{\pm j}$, $i, j = 1, 2, \dots$, are completely independent, with exponential, respectively, normal distributions:

$$\mathbf{P}\big(\xi_{\pm i} \in (x, x + \mathrm{d}x)\big) = 1\!\!1_{\{x \geq 0\}} e^{-x} \,\mathrm{d}x, \quad \mathbf{P}\big(\eta_{\pm j} \in (v, v + \mathrm{d}v)\big) = \frac{1}{\sqrt{2\pi}} e^{-v^2/2} \,\mathrm{d}v.$$

We shall consider two different types of particle systems in this paper. Their state spaces will be

$$\begin{aligned} \Omega^{I} &:= \{(\omega^+, \omega^-, z, u, V) : \omega^{\pm} \in \Omega^{\pm}, \quad z \in \mathbb{R}_+, \quad u \in [-1, 1], \quad V \in \mathbb{R}\}, \\ \Omega^{II} &:= \{(\omega^+, \omega^-, z) : \omega^{\pm} \in \Omega^{\pm}, \quad z \in \mathbb{R}_+\}. \end{aligned}$$

We also define the natural projection between these spaces:

$$\Pi : \Omega^{I} \to \Omega^{II}, \qquad \Pi(\omega^+, \omega^-, z, u, V) := (\omega^+, \omega^-, z).$$

In order to define the relevant probability measures on the state spaces Ω^{I} and Ω^{II} first we introduce some notation. Let the random variables W and ζ be independent and distributed as a standard Gaussian, respectively, as a standard $\Gamma(2)$. Let $\gamma_2(z)$ be the density of the distribution of ζ, $\varrho(c)$ the density of the distribution of $|W\zeta|$, and $\varphi_c(z)$

the density of the conditional distribution of ζ, given $|W\zeta| = c$:

$$\begin{aligned}
\gamma_2(z) &:= ze^{-z}, \\
\varrho(c) &:= \sqrt{\frac{2}{\pi}} \int_0^\infty \exp\{-z - \frac{c^2}{2z^2}\} \, \mathrm{d}z, \\
\varphi_c(z) &:= \frac{1}{\varrho(c)} \sqrt{\frac{2}{\pi}} \exp\{-z - \frac{c^2}{2z^2}\}.
\end{aligned}$$

Clearly,

$$\gamma_2(z) = \int_0^\infty \varphi_c(z) \varrho(c) \, \mathrm{d}c.$$

The probability measures considered on the state spaces Ω^I and Ω^{II} are $\mu^{I,M}$ (defined on Ω^I) which depends on the positive parameter M, respctively, $\mu^{II,c}$ (defined on Ω^{II}) which depends on the positive parameter c, and finally μ^{II} (also defined on Ω^{II}) which is a mixture of the measures $\mu^{II,c}$:

$$\begin{aligned}
\mu^{I,M}(\,\mathrm{d}\omega^I) &:= \mu^+(\,\mathrm{d}\omega^+) \times \mu^-(\,\mathrm{d}\omega^-) \times \gamma_2(z) \, \mathrm{d}z \times \frac{1}{2} \, \mathrm{d}u \times \sqrt{\frac{M}{2\pi}} e^{MV^2/2} \, \mathrm{d}V, \quad (1) \\
\mu^{II,c}(\,\mathrm{d}\omega^{II}) &:= \mu^+(\,\mathrm{d}\omega^+) \times \mu^-(\,\mathrm{d}\omega^-) \times \varphi_c(z) \, \mathrm{d}z, \quad (2) \\
\mu^{II}(\,\mathrm{d}\omega^{II}) &:= \mu^+(\,\mathrm{d}\omega^+) \times \mu^-(\,\mathrm{d}\omega^-) \times \gamma_2(z) \, \mathrm{d}z \\
&= \int_0^\infty \mu^{II,c}(\,\mathrm{d}\omega^{II}) \varrho(c) \, \mathrm{d}c. \quad (3)
\end{aligned}$$

The measures $\mu^{I,M}$, respectively, $\mu^{II,c}$ will be the natural Gibbs measures corresponding to the dynamics of our systems, to be defined in the next subsection.

2.2 Dynamics

We define the dynamics of the systems considered verbally, rather than writing formulas. The two types of dynamics considered will be called *of type I*, respectively, *of type II*. Their state spaces will be Ω^I, respectively, Ω^{II}. These will actually be families of dynamics parametrized by the fixed parameters $M > 0$, respectively, $c > 0$.

2.2.1 Dynamics of type I:

For precise formal definitions and basic facts about these dynamics see [14], [19], [20]. The system consists of particles indexed $\dots, -2, -1, 0, +1, +2, \dots$. The system is observed from the tagged particle of index 0. The tagged particle has mass M, the other particles have unit mass. Positions and velocities of the particles in the system are encoded in $(\omega^+, \omega^-, z, u, V)$ as follows: V is the velocity of the tagged particle, $x_{\pm i} \pm z(1 \pm u)/2$ and $v_{\pm i}$ is the position, respectively, the velocity of the particle of index $\pm i$, $i = 1, 2, \dots$. The

untagged gas particles perform uniform motion on the line and don't interact between themselves, when two of them meet and cross each other's trajectory they exchange their index. The tagged particle, while isolated from the others, also performs uniform motion and collides elastically at encounters with an untagged gas particle. At these collisions the outgoing velocities $V^{\text{out}}, v^{\text{out}}$ are determined by the incoming velocities $V^{\text{in}}, v^{\text{in}}$ as follows:

$$V^{\text{out}} = \frac{M-1}{M+1} V^{\text{in}} + \frac{2}{M+1} v^{\text{in}}, \qquad v^{\text{out}} = \frac{2M}{M+1} V^{\text{in}} - \frac{M-1}{M+1} v^{\text{in}}. \tag{4}$$

Mind that the untagged gas particles never exchange their order with the tagged particle and the index $\pm i$ of a particle denotes its actual relative order with respect to the tagged particle.

The measure $\mu^{I,M}$ defined in (1) is Gibbs measure for this dynamics, invariant for the system as seen from the tagged particle. It is a fact (see [14], [19], [20]) that the dynamics is $\mu^{I,M}$-a.s. well defined: starting the system distributed according to $\mu^{I,M}$, with probability 1 no multiple collisions will occur and the system remains locally finite indefinitely. We denote by $\mathcal{S}_t^{I,M}$ the measure preserving flow defined by this dynamics on $(\Omega^I, \mu^{I,M})$.

The velocity and displacement process of the tagged particle is

$$\begin{aligned} V_t^{I,M} &= V_t^{I,M}(\omega^I) := V(\mathcal{S}_t^{I,M}\omega^I) \\ Q_t^{I,M} &= Q_t^{I,M}(\omega^I) := \int_0^t V_s^{I,M}(\omega^I)\,\mathrm{d}s. \end{aligned}$$

In section 4 it will be more convenient to describe the dynamics from a fixed exterior point of observation. The absolute locations of the gas particles in the system as seen from such a fixed exterior frame of reference are

$$y_{\pm i}(t) := Q_t^{I,M} + x_{\pm i}(t), \quad \text{where} \quad x_{\pm i}(t) := x_{\pm i}(\mathcal{S}_t^{I,M}\omega^I), \qquad i = 1, 2, \dots. \tag{5}$$

We also introduce the variables

$$\begin{aligned} \widetilde{V}_t^{I,M} &= \widetilde{V}_t^{I,M}(\omega^I) := \frac{1}{2}\Big(v_{-1}(\mathcal{S}_t^{I,M}\omega^I) + v_{+1}(\mathcal{S}_t^{I,M}\omega^I)\Big) \\ \widetilde{Q}_t^{I,M} &= \widetilde{Q}_t^{I,M}(\omega^I) := \int_0^t \widetilde{V}_s^{I,M}(\omega^I)\,\mathrm{d}s. \end{aligned}$$

These are the velocity and position processes of the centre of mass of the particles next to the right and to the left of the tagged particle. We need the position process $\widetilde{Q}_t^{I,M}$ for later comparison with a similar process defined for the dynamics of type II in the next paragraph. Mind that the random process $t \mapsto \big(Q_t^{I,M} - \widetilde{Q}_t^{I,M}\big)$ is stationary and thus tight, uniformly for $t > 0$. As a consequence, $\big(Q_t^{I,M}/\sqrt{t} - \widetilde{Q}_t^{I,M}/\sqrt{t}\big) \to 0$ in $\mu^{I,M}$-probability (actually $\mu^{I,M}$-a.s.) as $t \to \infty$.

2.2.2 Dynamics of type II:

The system consists of particles of unit mass indexed $\dots,-2,-1,+1,+2,\dots$. Mind that there is no particle of index 0 in this system. The system is observed from the centre of mass of particles of index $+1$ and -1, we call this the central observation point. Positions and velocities of the particles in the system are encoded in (ω^+,ω^-,z) as follows: $x_{\pm i}\pm z/2$, respectively, $v_{\pm i}$ is the position relative to the central observation point, respectively, the velocity of the particle of index $\pm i$, $i=1,2,\dots$. Clearly, z denotes the distance between the two central particles of index $+1$ and -1. Particles move uniformly on the line except for the two central particles of index $+1$ and -1 which interact via the inverse quadratic pair potential $U(z)$, or equivalently repelling force $F(z)$:

$$U(z)=\frac{c^2}{2z^2}, \qquad F(z)=\frac{c^2}{z^3}, \tag{6}$$

where $c^2>0$ is a fixed parameter and z is the distance between the two central particles. When two gas particles meet and cross each other's trajectory they exchange their index. But mind that due to the strongly repulsive interaction between the two central particles, these two will never meet and thus particles will never change the sign of their index. The index $\pm i$ of a particle denotes its actual relative order with respect to the central observation point.

Remark. In the literature of completely integrable Hamiltonian systems the pair potential (6) is usually called Calogero-Moser-Sutherland interaction and leads to one of the most notorious completely integrable 1-d systems, see [5], [11] and [18] for the first original publications.

The measure $\mu^{II,c}$ defined in (2) is Gibbs measure for this dynamics, invariant for the system as seen from the centre of mass of the two central particles. It is again a fact that this dynamics is $\mu^{II,c}$-a.s. well defined. We denote by $\mathcal{S}_t^{II,c}$ the measure preserving flow defined by this dynamics on $(\Omega^{II},\mu^{II,c})$.

The velocity and displacement process of the point of observation is

$$\begin{aligned} V_t^{II,c}=V_t^{II,c}(\omega^{II}) &:= \frac{1}{2}\big(v_{-1}(\mathcal{S}_t^{II,c}\omega^{II})+v_{+1}(\mathcal{S}_t^{II,c}\omega^{II})\big)\\ Q_t^{II,c}=Q_t^{II,c}(\omega^{II}) &:= \int_0^t V_s^{II,c}(\omega^{II})\,\mathrm{d}s. \end{aligned}$$

Again, absolute locations of the gas particles in the system as seen from a fixed exterior frame of reference are expressed similarly to (5).

2.2.3 Stochastic processes considered

In this paper we consider the following *stochastic processes*:

$$\begin{aligned}
Q_t^{I,M} &= Q_t^{I,M}(\omega^I), \quad \text{with random } \omega^I \text{ distributed according to} \quad \mathrm{d}\mu^{I,M}, \\
\widetilde{Q}_t^{I,M} &= \widetilde{Q}_t^{I,M}(\omega^I), \quad \text{with random } \omega^I \text{ distributed according to} \quad \mathrm{d}\mu^{I,M}, \\
Q_t^{II,c} &= Q_t^{II,c}(\omega^{II}), \quad \text{with random } \omega^{II} \text{ distributed according to} \quad \mathrm{d}\mu^{II,c}, \\
Q_t^{II} &= Q_t^{II,c}(\omega^{II}), \quad \text{with random } (\omega^{II}, c) \text{ distributed according to} \quad \mathrm{d}\mu^{II,c}\varrho(c)\,\mathrm{d}c, \\
&= Q_t^{II,c}, \quad \text{with random } c \text{ distributed according to} \quad \varrho(c)\,\mathrm{d}c.
\end{aligned}$$

This means that the process Q_t^{II} is a $\varrho(c)\,\mathrm{d}c$-mixture of the processes $Q_t^{II,c}$

3 Survey of earlier results

In this section we summarize the old results – rigorously proved and numerical – regarding various limits for the motion of the tagged particle in the model of type I. In Section 4 we formulate and prove a new result concerning the $M \to 0$ behaviour of these systems. In Section 5 we describe our new numerical results, referring to this new model.

In all cases we are interested in the *diffusive scaling limit of the displacement of the tagged particle motion*, that is in the asymptotics of the rescaled process

$$t \mapsto A^{-1/2} Q_{At}, \qquad \text{as} \qquad A \to \infty.$$

Throughout the paper we denote by A this scaling parameter.

We shortly survey the existing results on the asymptotics of the tagged particle motion in model of type I in historical order. The constants

$$\underline{\sigma}^2 := \sqrt{\pi/8} \approx 0.627\ldots, \qquad \overline{\sigma}^2 := \sqrt{2/\pi} \approx 0.798\ldots$$

will play a key role in the formulation of these results.

3.1 The $M = 1$ case:

The case when the tagged particle has the same mass as the rest of the gas particles was investigated and solved in Spitzer (1969) [17]. For the roots of these ideas see also Harris (1965) [8]. In [17] the following invariance principle is proved:

$$\text{for } M = 1: \qquad A^{-1/2} Q_{At}^{I,M} \Rightarrow \overline{\sigma} W_t, \qquad \text{as} \qquad A \to \infty,$$

where $\Rightarrow$ stands for weak convergence of the sequence of *processes* (see [2] for weak convergence of processes), and W_t is a standard 1-d Borwnian motion. That is: $\overline{\sigma} W_t$ is a Brownian motion of variance $\overline{\sigma}^2$.

3.2 The Ornstein-Uhlenbeck limit:

Holley (1971) [9] considers the following limit when the mass of the tagged particle is rescaled in the same order as the time scale factor. Let $m \in (0, \infty)$ be fixed. Then

$$\text{for } M = mA: \qquad \left(A^{1/2} V_{At}^{I,M}, A^{-1/2} Q_{At}^{I,M}\right) \Rightarrow \left(\eta_t^m, \xi_t^m\right), \qquad \text{as} \qquad A \to \infty,$$

where η_t^m and ξ_t^m are the Ornstein-Uhlenbeck velocity, respectively, position processes defined by the SDEs

$$\mathrm{d}\eta_t^m = -\gamma(m)\eta_t^m \,\mathrm{d}t + \sqrt{D(m)}\,\mathrm{d}W_t, \quad \xi_t^m = \int_0^t \eta_s^m ds,$$

with friction and dispertion parameters

$$\gamma(m) := \frac{4}{m}\sqrt{\frac{2}{\pi}}, \quad D(m) := \frac{8}{m^2}\sqrt{\frac{2}{\pi}}.$$

For a version in higher dimensions of this type of result see Dürr, Goldstein, Lebowitz (1981) [6].

It is important to remark (see [20]), that

$$\xi_t^m \Rightarrow \underline{\sigma} W_t, \qquad \text{as} \qquad m \to 0.$$

This means that taking first Holley's limit, then $m \to 0$ we obtain a Wiener process of variance $\underline{\sigma}^2$ as the diffusive scaling limit of the displacement of the tagged particle.

3.3 Bounds for the limiting variance for any M:

Sinai, Soloveichik (1986) [14], respectively, Szász, Tóth (1986) [19] consider the case of arbitrary fixed mass M of the tagged particle. In these papers very similar rersults are proved in completely different ways. The results are summarized as follows:

$$\text{for } M \ll A: \qquad \underline{\sigma}^2 t \le \liminf_{A \to \infty} \mathbf{Var}\left(A^{-1/2} Q_{At}^{I,M}\right) \le \limsup_{A \to \infty} \mathbf{Var}\left(A^{-1/2} Q_{At}^{I,M}\right) \le \overline{\sigma}^2 t.$$

Mind that these bounds are *independent of the mass of the tagged particle*. For surveys of these results see also [13], [15], [16], [21].

Any rigorous result regarding the mass dependence of the limiting variance

$$\sigma_M^2 := \lim_{t \to \infty} \mathbf{Var}\left(t^{-1/2} Q_t^{I,M}\right)$$

remains one of the most interesting open questions in this context till today. The only known case is Spitzer's result $\sigma_1 = \overline{\sigma}$. For numerical results see subsection 3.5 below.

3.4 Large mass Wiener limit:

In order to interpolate between the M = const. cases (see subsection 3.3) and Holley's limit (see subsection 3.2,) Szász and Tóth (1987) [20] considered the limit with asymptotics $1 \ll M \ll A$, as $A \to \infty$. Here the main result is the following invariance principle:

$$\text{for } A^{1/2+\varepsilon} \ll M \ll A: \qquad A^{-1/2} Q^{I,M}_{At} \Rightarrow \underline{\sigma} W_t, \quad \text{as} \quad A \to \infty. \tag{7}$$

Actually, the scaling limit (7) should hold for $1 \ll M \ll A$ but the method of proof in [20] based on a coupling argument breaks down for $1 \ll M \ll A^{1/2+\varepsilon}$. For a survey of the results recalled in this and the previous paragraph see also [21].

3.5 Earlier numerical results

Following [14] and [19] various numerical investigations were performed in order to establish the mass dependence of the limiting variance: $M \mapsto \sigma^2_M$.

The relevant numerical investigations performed in the late eighties, early nineties are published in Omerti, Ronchetti, Dürr (1986) [12], Khazin (1987) [10], Boldrighini, Cosimi, Frigio (1990) [3], Fernandez, Marro (1993) [7]. These results clearly suggest the qualitative dependence $M \mapsto \sigma^2_M$ shown in Figure 1.

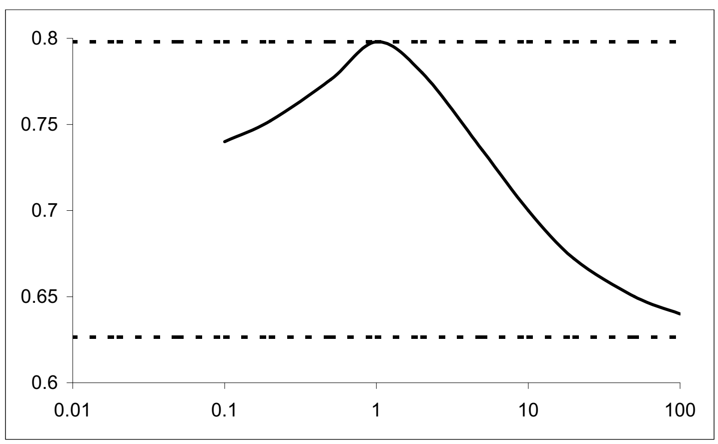

Figure 1: Qualitative dependence $M \mapsto \sigma^2_M$ suggested by earlier numerical works

As about the $M \to 0$ limit: in all these papers it is remarked that the numerical simulations for small mass of the tagged particle are unreliable due to instability. On the other hand there was agreement between all researchers intrested in these questions

that $\lim_{M\to 0}\sigma_M^2 = \overline{\sigma}^2 \approx 0.798\ldots$ should hold. The "starightforward argument" was the following: the tagged particle of extremely small mass must have very small effect on the system, vanishing as $M \to 0$. So, in the $M \to 0$ limit the displacement of any marked particle (in particular the one next to the right of the tagged particle) will asymptotically behave exactly like the tagged particle in Spitzer's equal mass case, cf. subsection 3.1, above. So, the more recent and more accurate numerical results published in Boldrighini, Frigio, Tognetti (2002) [4], suggesting that

$$\lim_{M\to 0}\sigma_M^2 =: \sigma_0^2 \approx 0.74\ldots \tag{8}$$

which is *strictly* inbetween $\underline{\sigma}^2 \approx 0.627\ldots$ and $\overline{\sigma}^2 \approx 0.798\ldots$, *came as a surprise.*

The results of the present note provide substantial theoretical and independent numerical support of this surprising fact.

4 The $M \to 0$ limit of dynamics of type I

Theorem 1. *Let $z \in \mathbb{R}^+$, $u \in [-1,1]$, $W \in \mathbb{R}$ be fixed, $M_n \to 0$, $V_n = M_n^{-1/2}W_n$ so that $W_n \to W \in \mathbb{R}$, and define $c := |Wz|$. Choose $\omega^\pm \in \Omega^\pm$ so that for all n the dynamic trajectories $\mathcal{S}_t^{I,M_n}(\omega^+,\omega^-,z,u,V_n)$ and $\mathcal{S}_t^{II,c}(\omega^+,\omega^-,z)$ are well defined for all $t \in [0,\infty)$. (Mind that for any choice of z, u, W and sequences M_n, V_n these $\omega^\pm$-s are of full $\mu^\pm$ measure in $\Omega^\pm$.) Then for all $t \in [0,\infty)$*

$$\lim_{n\to\infty} \Pi\mathcal{S}_t^{I,M_n}(\omega^+,\omega^-,z,u,V_n) = \mathcal{S}_t^{II,c}(\omega^+,\omega^-,z).$$

The convergence is uniform on compact intervals of time.

Proof. Within this proof it is convenient to describe the systems of particles as seen from a fixed external frame of reference: the postion of the tagged particle (in the system of type I) at time t is $Q_t^{I,M}$, the postitions of the untagged gas particles are $y_{\pm i}(t)$, $i = 1,2,\ldots$, as given in (5).

We have to prove that in the limit described in the theorem the trajectories of the particles in system I converge to the coresponding trajectories in the limit system of type II. Note that the particles with $i \neq \pm 1, 0$ follow the same dynamical rules in the two types of dynamics. Thus we only need to understand how the motion of the particles with indices ± 1 can be approximated as $M \to 0$, if they interact with the tagged particle according to the rules of section 2.2.1.

As mentioned above, the particles with indices -1, 0 and 1 have positions $y_{-1}(t) \leq Q_t \leq y_1(t)$ and velocities v_{-1}, $V_t = W_t/\sqrt{M}$ and $v_1(t)$, respectively, where $v_{\pm 1}$ and W are of order one. As V is very large, the tagged particle performs a full cycle: hits one of its neighbours, turns back, collides with the other neighbour, and gets back to its initial position within a very short time $\mathrm{d}t$. See Fig 2 for insight.

To investigate how the system evolves in this time interval $\mathrm{d}t$, two successive collisions should be taken into account. We may assume that $W > 0$ (the case of negative W is

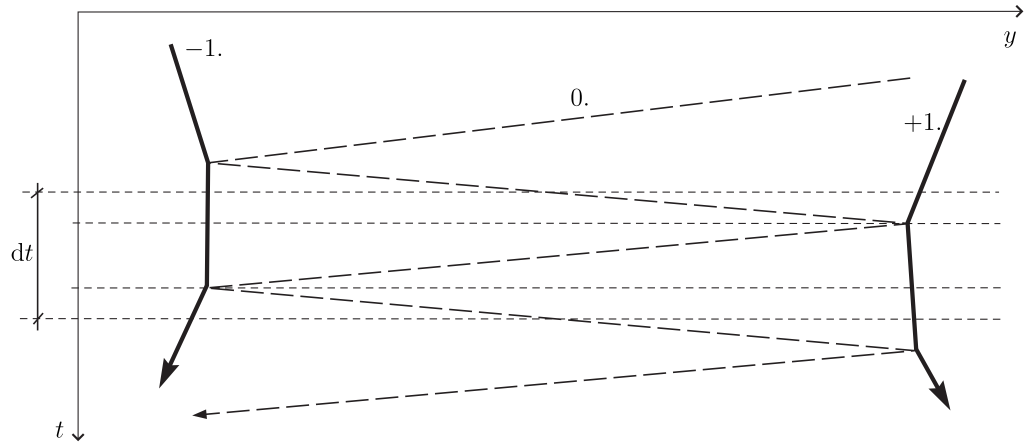

Figure 2: Successive collisions of the tagged particle of mass $M \ll 1$ with its neighbours

analogous), and thus the tagged particle collides first with the particle of index 1, and then with that of index -1. These collisions split the time interval into three smaller subintervals. Let us expand the formulas of (4) in the limit as $M \to 0$. This way we may calculate the velocities of the three particles in the three subintervals, see Table 1. Mind that the order of magnitude of the incoming velocities are as follows

$$V = W/\sqrt{M} \asymp M^{-1/2}, \qquad v_{\pm 1} \asymp 1.$$

	1. interval	2. interval	3. interval
particle 1	v_1	$v_1 + 2MV + \mathcal{O}(M)$	$v_1 + 2MV + \mathcal{O}(M)$
particle 0	V	$-V + 2v_1 + \mathcal{O}(\sqrt{M})$	$V - 2v_1 + 2v_{-1} + \mathcal{O}(\sqrt{M})$
particle -1	v_{-1}	v_{-1}	$v_{-1} - 2MV + \mathcal{O}(\sqrt{M})$

Table 1: Velocities in the $M \to 0$ approximation

In particular, the tagged particle reverts its velocity at collisions, thus its speed is constant, more precisely, equal to $|V| + \mathcal{O}(1) = |W/\sqrt{M}| + \mathcal{O}(1)$ throughout the investigated time interval. This implies $dt \asymp \sqrt{M}$. Furthermore, the velocities v_1 and v_{-1} remain $\mathcal{O}(1)$, and thus, the particles of index 1 and -1 remain $\mathcal{O}(\sqrt{M})$-close to their original positions y_1 and y_{-1} in the investigated interval. In accordance with the notations of subsection 2.1, let us introduce $z = y_1 - y_{-1}$ for brevity. By the above observations

the distance of the two non-tagged particles remains $\mathcal{O}(\sqrt{M})$-close to z. Now we may calculate the leading term in $\mathrm{d}t$:

$$\mathrm{d}t = \frac{2z + \mathcal{O}(\sqrt{M})}{V + \mathcal{O}(1)} = \frac{2z}{W}\sqrt{M} + \mathcal{O}(M). \tag{9}$$

Let us denote the amount with which the velocities change at the collisions (and thus, during the studied time interval) by $\mathrm{d}v_1$ and $\mathrm{d}v_{-1}$.

Referring to Table 1 we get

$$\mathrm{d}v_1 = 2W\sqrt{M} + \mathcal{O}(M), \qquad \mathrm{d}v_{-1} = -2W\sqrt{M} + \mathcal{O}(M). \tag{10}$$

Formulas (9) and (10) altogether imply that, as $M \to 0$, $v_1(t)$ and $v_{-1}(t)$ approach (piecewise) differentiable functions, and

$$\dot{v}_1 = \frac{W^2}{z}, \qquad \dot{v}_{-1} = -\frac{W^2}{z}. \tag{11}$$

Referring again to Table 1, we may calculate the amount of change in the velocity of the tagged particle during the time interval $\mathrm{d}t$. We get

$$\mathrm{d}V = 2v_{-1} - 2v_1 + \mathcal{O}(\sqrt{M}), \qquad \text{thus} \qquad \mathrm{d}W = \sqrt{M}(2v_{-1} - 2v_1) + \mathcal{O}(M). \tag{12}$$

Formulas (9) and (12) altogether imply

$$\dot{W} = -\frac{(v_1 - v_{-1})W}{z} = -\frac{\dot{z}W}{z},$$

where we have used that $v_1 - v_{-1} = \dot{y}_1 - \dot{y}_{-1} = \dot{z}$.

Integrating this differential equation we find that $|Wz|$ is an integral of motion. This means that in the $M \to 0$ limit, $c = |W(t)z(t)|$ is *constant* during a time interval when the tagged particle has the same neighbours, and within such an inverval, (11) gives that the positions and velocities for the particles with indices ± 1 satisfy the coupled differential equations

$$\begin{aligned} \dot{x}_1 &= v_1, & \dot{v}_1 &= c^2/z^3, \\ \dot{x}_{-1} &= v_{-1}, & \dot{v}_{-1} &= -c^2/z^3. \end{aligned}$$

This is in agreement with the formula (6) for the potential describing the systems of type *II*.

Notice now that the value of $c = |W(t)z(t)|$ also remains constant when one of the neighbours of the tagged particle 'meets' another gas particle, and the neighbour is replaced by that new particle. At such a time moment the values of both W and z are unchanged. Thus for any $t > 0$ $|W(t)z(t)| = |W(0)z(0)| = c$ according to the choice of c in the formulation of Theorem 1. This completes the proof of Theorem 1. □

Remark. Note that taking the $c \to 0$ limit of the dynamics of type II, we recover the dynamics of type I with equal masses: the interaction between the two central particles becomes hard core specular collision. So, in this double limit ($M \to 0$ and than $c \to 0$)) the system behaves indeed as Spitzer's model, see subsection 3.1.

Recall that according to (3) the measure μ^{II} which is the projection of the measures $\mu^{I,M}$ on the state space Ω^{II}, is the $\varrho(c)\,\mathrm{d}c$-mixture of the Gibbs measures $\mu^{II,c}$. This implies that Theorem 1 has the following immediate corollary:

Corollary. *Let $M \to 0$. For any fixed $0 < T < \infty$, the sequence of processes $[0,T] \ni t \mapsto \widetilde{Q}_t^{I,M}$ converges weakly (in distribution) to the process to $[0,T] \ni t \mapsto Q_t^{II}$.*

5 Numerical results on systems of type II

5.1 Generalities

In this section we describe numerical investigations aimed at calculating the limiting variance

$$\sigma^2 := \lim_{t\to\infty} t^{-1}\mathbf{Var}\big(Q_t\big)$$

for the systems of type II. We shall also comment on how these results are related to the $M \to 0$ limit of the variance for the systems of type I, as established numerically in [4].

These simulations of the systems of type II were done by following a number of particles for some fixed time T. The particles followed were those who were less than $10T$ far away from the point of observation in the beginning. It is easy to check that with this method the probability of not following a particle that would indeed participate in the interaction, is negligible in all the cases we looked at.

Numerial simulation of the dymanics of type II is relatively fast, since the equation of motion for the two particles interacting via the potential (6) can be solved explicitly. (This observation is at the heart of the complete solvability of the Calogero-Moser-Sutherland model.)

The simulation for time T was repeated over a sample of N initial conditions chosen independently according to the appropriate stationary Gibbs distribution. From this sample, the empirical variance was calculated for $\mathbf{Var}\big(Q_t\big)$ as a function of t.

The result of a typical simulation can be seen in Figure 3. The solid line is the best linear fit for the tail, while the dashed lines have slope $\underline{\sigma}^2$ and $\overline{\sigma}^2$, and are drawn for comparison.

As we can see, $\mathbf{Var}\big(Q_t\big)$ does appear to be asymptotically linear. To read the limit $\lim_{t\to\infty} t^{-1}\mathbf{Var}\big(Q_t\big)$ from the graph, we needn't perform such a long simulation, during which this limit is well approached: the slope of the asymptote can be found with a good accuracy much sooner. Thus all the limits given in the paper are obtained using this technique, and the time interval for the simulation is typically between $T = 10$ and

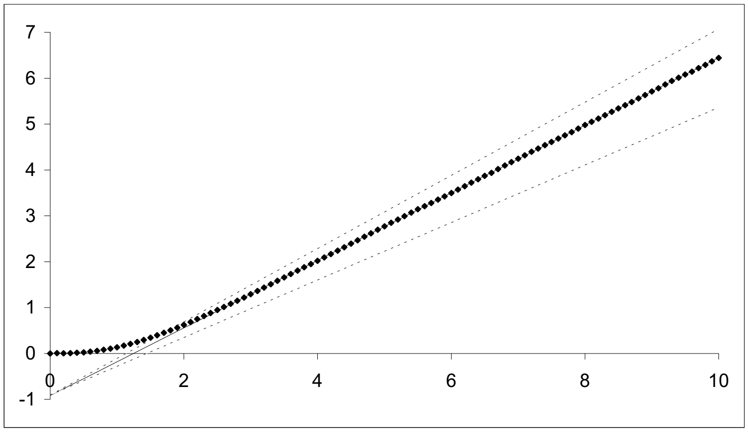

Figure 3: $\mathbf{Var}\big(Q_t\big)$ as a function of t in a typical simulation

$T = 50$. In exchange, the size of the sample can be very big – actually, samples up to $N = 10^7$ were used.

Finally, the statistical error of the calculated values was estimated by simply repeating the whole procedure about 20 times and calculating the standard deviation of the values obtained.

A detailed description of the numerical simulation and the source code for the applied program can be found in [22].

5.2 The systems with fixed c

We simulated numerically the dynamics of type II for various fixed values of the parameter c ranging between 0.01 and 100. We started the system from samples of the stationary Gibbs distribution $\mu^{II,c}$ and computed the limiting variance

$$\sigma_c^2 := \lim_{t\to\infty} t^{-1}\mathbf{Var}\big(Q_t^{II,c}\big).$$

We found the $c \mapsto \sigma_c^2$ dependence of the limiting variance as shown in Figure 4. We see that $\lim_{c\to 0}\sigma_c^2 \to \overline{\sigma}^2$, which is no surprise, since in the $c \to 0$ limit the system indeed behaves like the system of type I with $M = 1$, which is known to have $\sigma_{M=1}^2 = \overline{\sigma}^2$. See subsection 3.1 and the Remark after the proof of Theorem 1.

On the other hand, it is interesting to see that as $c \to \infty$, the limiting variance decreases, and even seems to approach a value near the lower limit $\underline{\sigma}^2$, but not quite reaching this lower bound. We plan to return to this phenomenon in the forthcoming paper [1].

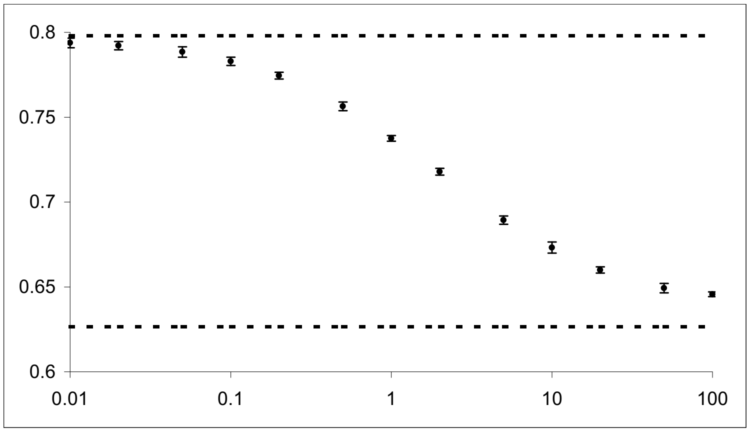

Figure 4: c-dependence of the limiting variance for systems of type II

5.3 The mixed system

We computed the numerical value of the limiting variance for the mixture of dynamics in two different ways.

First, we computed numerically the value of

$$\sigma^2_{\text{mix},1} := \lim_{t\to\infty} t^{-1}\mathbf{Var}\big(Q_t^{II}\big).$$

We have done it in the following way: we sampled the initial conditions ω^{II} according to the distribution μ^{II} and, independently, a standard normal variable W. Then we computed $c := |Wz|$, where z was the distance between the two central particles in the initial configuration ω^{II}. This *random* value c served as strength parameter in the interaction potential (6), with which the dynamics $\mathcal{S}_t^{II,c}$ was computed.

Second, using the data obtained for σ_c^2 in the fixed c computations (see subsection 5.2), we computed the mixture

$$\sigma^2_{\text{mix},2} := \int_0^\infty \sigma_c^2 \rho(c)\,\mathrm{d}c,$$

which, of course, in principle must give the same value as the previous computation.

Indeed, in the two cases we obtained the numerical values

$$\sigma^2_{\text{mix},1} = 0.736 \pm 0.003, \quad \sigma^2_{\text{mix},2} = 0.740 \pm 0.003.$$

This result is very interesting, since it coincides exactly (well within statistical error) with the $M \to 0$ limit of the variance calculated numerically in [4], see (8). This means that there is indeed *continuity* in the limiting variance as $M \to 0$.

We remark that the function $c \mapsto \sigma_c^2$ shown in Figure 4 can be fit with amazing accuracy by the function of the simple form $\sigma_c^2 = \frac{A_1 - A_2}{1+\left(\frac{c}{c_0}\right)^p} + A_2$, where $A_1 = 0.796$, $A_2 = 0.638$, $c_0 = 1.981$, $p = 0.792$.

Acknowledgement. We thank Henk van Beijeren for pointing out the relation of our result with the Calogero-Moser-Sutherland interaction. The research work of the authors is partially supported by the following OTKA (Hungarian National Research Fund) grants: F 60206 (for P.B.), K 60708 (for B.T.), T 46187 (for P.T.) and TS 49835 (for P.B. and P.T.); and by the Bolyai scholarship of the MTA (for P.B.).

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[22] Description of the numerical simulation and program code available online at `http://www.renyi.hu/~mogy/publications/szimulacio/brown1d`

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